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Regularization, Pseudofunction, and Hadamard Finite Part

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First, we discuss and correlate the various types of regularizations available in the literature for the singular function $H(x)/x^k$, where k is an integer and $H(x)$ is the Heaviside function. Then we present the corresponding regularization for the function r^{-k} , where r is the radial distance in \mathbb{R}^n . Thereafter, we express the recently discovered distributional derivatives of this function in terms of pseudofunctional language commonly used in the Coulomb, gravitational, and interparticle potentials where the function $1/r$ plays a fundamental role. © 1989 Academic Press, Inc.

1. INTRODUCTION

The singular function $H(x)/x^k$, where k is an integer (defined in the abstract), arises in many mathematical and physical problems. Various regularization procedures are available for this function in the literature. In this paper we discuss the relationship among these regularizations. The function $1/r^k$, where r is the radial distance, also arises in various mathematical and physical problems. However, all the corresponding regularizations of this function are not available in the literature. We present them and discuss their relationships.

We have recently presented [1] an explicit expression for the general N th-order distributional derivative of $1/r^k$ in \mathbb{R}^n . Since the regularization used by us is different from the one used in the study of pseudofunctions, it is causing some difficulties to the readers in physical sciences where the function $1/r$ plays an important part. The relationships between various

regularizations of the function $1/r^k$ as presented in this paper enable us to remove these difficulties. Indeed, we derive the expression for the general N th-order derivative for the pseudofunction $1/r^k$, the regularization commonly used in modern physics.

2. THE VARIOUS REGULARIZATION OF $H(x)/x^k$

As is well known [2-7] a function of n variables having a single algebraic singularity of order k at the point $\mathbf{a} = (a_1, \dots, a_n)$ (k is the smallest integer with the property that $\|\mathbf{x} - \mathbf{a}\|^k f(\mathbf{x})$ is integrable near $\mathbf{x} = \mathbf{a}$) admits distributional regularizations of the order k , that is, there are distributions $\tilde{f}(\mathbf{x})$ such that

$$\langle \tilde{f}(\mathbf{x}), \phi(\mathbf{x}) \rangle = \int_{\mathbb{R}^n} f(\mathbf{x}) \phi(\mathbf{x}) d\mathbf{x}, \quad (2.1)$$

whenever ϕ is a test function that satisfies

$$\mathbf{D}^{(\alpha_1, \dots, \alpha_n)} \phi|_{\mathbf{x}=\mathbf{a}} = \frac{\partial^{|\alpha|} \phi}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}} \Big|_{\mathbf{x}=\mathbf{a}} = 0, \quad |\alpha| = \alpha_1 + \dots + \alpha_n \leq k-1. \quad (2.2)$$

Unfortunately, regularizations of order k are not unique, since if \tilde{f} is one such regularization then so is

$$\tilde{f}(\mathbf{x}) + \sum_{|\alpha| \leq k-1} b_\alpha D^\alpha \delta(\mathbf{x} - \mathbf{a}), \quad (2.3)$$

for any choice of the constants b_α , $|\alpha| = \alpha_1 + \dots + \alpha_n \leq k-1$. There is no regularization procedure satisfying natural continuity requirements that can be used to obtain the regularization of all functions with algebraic singularities of the order k . Special regularization procedures are available for certain classes of functions (powers of $\|\mathbf{x} - \mathbf{a}\|$, logarithms, etc.), but unfortunately the results vary from author to author.

Our aim is to present the relationships among the various regularizations of $H(x)/x^k$, where $H(x)$ is the Heaviside function, and of the powers of the inverse radial function $1/r^k$, $r = (x_1^2 + \dots + x_n^2)^{1/2}$, and to give the corresponding formulas for their derivatives of arbitrary order.

As is clear from the non-uniqueness of regularizations, the usual properties of the ordinary functions may or may not hold for their regularizations. Among the properties of the functions $H(x)/x^k$ we would like to point out the following:

$$x^q \frac{H(x)}{x^k} = \frac{H(x)}{x^{k-q}}, \quad 0 \leq q \leq k \quad (2.4)$$

$$\frac{d}{dx} \left(\frac{H(x)}{x^k} \right) = -k \frac{H(x)}{x^{k+1}}, \quad (2.5)$$

$$\frac{d}{dx} (H(x) \ln x) = \frac{H(x)}{x}. \quad (2.6)$$

It is interesting to observe that there are no regularizations for which the generalized versions of (2.4)–(2.6) hold simultaneously. However, there are several regularizations for which both (2.4) and (2.6) hold and there is precisely one regularization for which both (2.5) and (2.6) hold.

The regularizations $R_1(H(x)/x^k)$ used in [1] are defined as

$$R_1 \left(\frac{H(x)}{x} \right) = \frac{\bar{d}}{dx} (H(x) \ln x), \quad (2.7a)$$

$$R_1 \left(\frac{H(x)}{x^{k+1}} \right) = -\frac{1}{k} \frac{\bar{d}}{dx} \left(\frac{H(x)}{x^k} \right), \quad k \geq 0, \quad (2.7b)$$

where the bar indicates a generalized derivative. Formula (2.4) does not hold for these regularizations, since as is shown in that reference we have

$$x^q R_1 \left(\frac{H(x)}{x^k} \right) = R_1 \left(\frac{H(x)}{x^{k-q}} \right) - \frac{(-1)^{k-q-1}}{(k-q-1)!} (\psi(k) - \psi(k-q)) \delta^{(k-q-1)}(x), \quad (2.8)$$

for $k \geq q+1$. Here we use the classical notation [8]

$$\psi(k) = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + 1/k - 1 - \gamma = \frac{d}{dz} (\ln \Gamma(z))|_{z=k}, \quad (2.9)$$

where $\gamma = -\Gamma'(1)$ is Euler's constant. We warn the reader that other notations have been used in the literature, for instance, in [1] $\psi(k)$ denotes the partial sum $1 + \frac{1}{2} + \cdots + 1/k$, while Jones [3] denotes by $\psi(k)$ the quantity $1 + \frac{1}{2} + \cdots + 1/k - \gamma$.

Another method of regularization is provided by Hadamard's finite part. The idea of this method is the following. Suppose we want to assign a meaning to the divergent integral

$$\int_0^\infty \frac{\phi(x)}{x^k} dx, \quad (2.10)$$

where $\phi \in \mathcal{D}(\mathbb{R})$, the space of infinitely differentiable functions of compact support. Then we consider the integral

$$F(\varepsilon) = \int_{\varepsilon}^{\infty} \frac{\phi(x) dx}{x^k}. \quad (2.11)$$

It is not hard to show that $F(\varepsilon)$ has the form

$$F(\varepsilon) = F_0(\varepsilon) + a_0 \ln \varepsilon + \sum_{j=1}^{k-1} a_j / \varepsilon^j, \quad (2.12)$$

for some constants a_0, \dots, a_{k-1} and a function $F_0(\varepsilon)$ that has a finite limit when $\varepsilon \rightarrow 0$. The *finite part in the sense of Hadamard* is defined as $\lim_{\varepsilon \rightarrow 0} F_0(\varepsilon)$.

Since the form (2.12) depends on the analytical character of the function $H(x)/x^k$, the finite part method cannot be used to assign a meaning to a general divergent integral of the form $\int_{-\infty}^{\infty} f(x) \phi(x) dx$.

The computation of the finite part of the integral (2.10) can be performed by dividing the interval of integration in (2.11) and by adding and subtracting an appropriate term:

$$\begin{aligned} \int_{\varepsilon}^{\infty} \frac{\phi(x)}{x^k} dx &= \int_a^{\infty} \frac{\phi(x)}{x^k} dx + \int_{\varepsilon}^a \frac{1}{x^k} \left[\phi(x) - \sum_{j=0}^{k-1} \frac{\phi^{(j)}(0)}{j!} x^j \right] dx \\ &\quad + \int_{\varepsilon}^a \sum_{j=0}^{k-1} \frac{\phi^{(j)}(0)}{j!} x^{j-k} \\ &= \int_a^{\infty} \frac{\phi(x)}{x^k} dx + \int_{\varepsilon}^a \frac{1}{x^k} \left[\phi(x) - \sum_{j=0}^{k-1} \frac{\phi^{(j)}(0)}{j!} x^j \right] dx \\ &\quad - \sum_{j=0}^{k-2} \frac{\phi^{(j)}(0)}{j!(k-j-1)} \left[\frac{1}{a^{k-j-1}} - \frac{1}{\varepsilon^{k-j-1}} \right] \\ &\quad + \frac{\phi^{(k-1)}(0)}{(k-1)!} (\ln a - \ln \varepsilon), \end{aligned}$$

therefore the finite part of the integral is

$$\begin{aligned} Fp \int_0^{\infty} \frac{\phi(x)}{x^k} dx &= \int_a^{\infty} \frac{\phi(x)}{x^k} dx + \int_0^a \frac{1}{x^k} \left[\phi(x) - \sum_{j=0}^{k-1} \frac{\phi^{(j)}(0)}{j!} x^j \right] dx \\ &\quad - \sum_{j=0}^{k-2} \frac{\phi^{(j)}(0)}{j!(k-j-1) a^{k-j-1}} + \frac{\phi^{(k-1)}(0)}{(k-1)!} \ln a, \quad (2.13) \end{aligned}$$

where Fp indicates the finite part. Observe that the result in (2.13) does not

depend on the value of the constant a ; it is usual to take $a = 1$. We denote the regularization of $H(x)/x^k$ obtained in this fashion as $Pf(H(x)/x^k)$.

Using integration by parts it is easy to show that

$$\frac{d}{dx} (\ln x H(x)) = Pf\left(\frac{H(x)}{x}\right), \quad (2.14a)$$

$$\frac{d}{dx} \left(Pf\left(\frac{H(x)}{x^k}\right) \right) = -k Pf\left(\frac{H(x)}{x^{k+1}}\right) + \frac{(-1)^k \delta^{(k)}(x)}{k!}. \quad (2.14b)$$

Comparison with (2.7a), (2.7b) yields the formulas

$$Pf\left(\frac{H(x)}{x}\right) = R_1\left(\frac{H(x)}{x}\right), \quad (2.15a)$$

$$Pf\left(\frac{H(x)}{x^k}\right) = R_1\left(\frac{H(x)}{x^k}\right) + \frac{(-1)^{k-1}}{(k-1)!} (\psi(k) + \gamma) \delta^{(k-1)}(x). \quad (2.15b)$$

Next, if we use (2.8), (2.15a) and (2.15b) we obtain

$$x^q Pf\left(\frac{H(x)}{x^k}\right) = Pf\left(\frac{H(x)}{x^{k-q}}\right), \quad q: 0, 1, \dots, k-1. \quad (2.16)$$

If we now put $a = \varepsilon$ in (2.13) and let ε approach zero, we obtain the truncated asymptotic form

$$Pf\left(\frac{H(x)}{x^k}\right) = \lim_{\varepsilon \rightarrow 0} \left[\frac{H(x-\varepsilon)}{x^k} - \sum_{j=0}^{k-2} \frac{(-1)^j \delta^{(j)}(x)}{j!(k-j-1) \varepsilon^{k-j-1}} + \frac{(-1)^{k-1}}{(k-1)!} \ln \varepsilon \delta^{(k-1)}(x) \right]. \quad (2.17)$$

This agrees with the result given by us [1],

$$R_1\left(\frac{H(x)}{x^k}\right) = \lim_{\varepsilon \rightarrow 0} \left[\frac{H(x-\varepsilon)}{x^k} - \sum_{j=0}^{k-2} \frac{(-1)^j \delta^{(j)}(x)}{j!(k-j-1) \varepsilon^{k-j-1}} - \frac{(-1)^{k-1}}{(k-1)!} (\psi(k) + \gamma - \ln \varepsilon) \delta^{(k-1)}(x) \right], \quad (2.18)$$

when (2.15) is taken into account.

A somewhat different regularization procedure is based upon the concept of analytic continuation. When λ is a complex number with $\text{Re } \lambda > -1$, the function $H(x)x^\lambda$ is locally integrable near $x=0$ and it therefore defines a

regular distribution, usually denoted by x_+^λ . Since x_+^λ is an analytic (generalized) function of λ and since

$$\frac{d}{dx} (x_+^\lambda) = \lambda x_+^{\lambda-1}, \quad \text{Re } \lambda > 0, \quad (2.19)$$

we can construct the analytical continuation of x_+^λ to the region $\mathbb{C} \setminus \{-1, -2, -3, \dots\}$ by using the definition

$$x_+^\lambda = \frac{1}{(\lambda+n)(\lambda+n-1)\cdots(\lambda-1)} \frac{d^n}{dx^n} (x_+^{\lambda+n}), \quad (2.20)$$

where n is any positive integer with $n + \text{Re } \lambda > -1$. In this fashion we obtain a regularization x_+^λ of $H(x)x^\lambda$ when $\text{Re } \lambda \leq -1$, $\lambda \neq -1, -2, -3, \dots$.

It is easy to show that the usual formulas such as

$$x^n x_+^\lambda = x_+^{\lambda+n}, \quad (2.21)$$

$$\frac{d}{dx} (x_+^\lambda) = \lambda x_+^{\lambda-1} \quad (2.22)$$

remain valid. In this sense x_+^λ is the canonical regularization of $H(x)x^\lambda$.

Unfortunately, the analytic function x_+^λ has poles at the points $\lambda = -1, -2, -3, \dots$ and this leads to the non-uniqueness of the regularization of $H(x)/x^k$. In fact, it is easy to see that all the poles are simple and that the residues are given by

$$\text{Res}_{\lambda=-k} x_+^\lambda = \frac{(-1)^{k-1}}{(k-1)!} \delta^{(k-1)}(x). \quad (2.23)$$

Even though the function x_+^λ does not have a limit when λ approaches a negative integer $-k$, a finite result is obtained by subtracting the singular part. This leads to a regularization of $H(x)/x^k$ that turns out to be equal to the finite part regularization:

$$Pf\left(\frac{H(x)}{x^k}\right) = \lim_{\lambda \rightarrow -k} \left[x_+^\lambda - \frac{(-1)^{k-1}}{(k-1)!} \delta^{(k-1)}(x) \right]. \quad (2.24)$$

Yet another possible regularization method is available, namely, if $a > 0$, a regularization of a function $f(x)$ with an algebraic singularity of order k at the origin is defined by

$$\langle \text{Reg}_a(f(x)), \phi(x) \rangle = \int_{-\infty}^{\infty} f(x) \left\{ \phi(x) - \left[\sum_{j=0}^{k-1} \frac{\phi^{(j)}(0)}{j!} x^j \right] H(a^2 - x^2) \right\} dx. \quad (2.25)$$

Observe that the result depends on the value of a . From (2.13) it easily follows that

$$\begin{aligned} \text{Reg}_a \left(\frac{H(x)}{x^k} \right) = Pf \left(\frac{H(x)}{x^k} \right) + \sum_{j=0}^{k-2} \frac{(-1)^j \delta^{(j)}(x)}{j!(k-j-1) a^{k-j-1}} \\ - \frac{(-1)^{k-1} \delta^{(k-1)}}{(k-1)!} \ln a. \end{aligned} \quad (2.26)$$

It is interesting to observe that if $a=1$, the regularizations $\text{Reg}_1(H(x)/x^k)$ satisfy (2.4) and (2.6).

3. THE VARIOUS REGULARIZATIONS OF r^{-k} IN \mathbb{R}^n

The various regularization procedures explained to obtain the regularizations of $H(x)/x^k$ can be applied to obtain regularizations of $r^{-k} = (x_1^2 + \dots + x_n^2)^{-k/2}$ in the space $\mathcal{D}'(\mathbb{R}^n)$, the space dual to $\mathcal{D}(\mathbb{R}^n)$. That is, we can consider the Hadamard's finite part of the divergent integral $\int_{\mathbb{R}^n} r^{-k} \phi(\mathbf{x}) d\mathbf{x}$, or consider the limit of the regular part of the generalized analytic function r^λ when λ approaches an integer.

The approach suggested in (2.25) can be generalized to the n -dimensional situation as follows. Let A be a measurable set of finite measure such that $\mathbf{0}$ belongs to its interior $\overset{\circ}{A}$, then a function of n variables $f(\mathbf{x})$ having a single algebraic singularity of order k at $\mathbf{x} = \mathbf{0}$ admits the regularization

$$\langle \text{Reg}_A(f(\mathbf{x})), \phi(\mathbf{x}) \rangle = \int_{\mathbb{R}^n} f(\mathbf{x}) \left\{ \phi(\mathbf{x}) - \left[\sum_{|\alpha| \leq k-1} \frac{\mathbf{D}^\alpha \phi(\mathbf{0})}{\alpha!} \mathbf{x}^\alpha \right] H_A(\mathbf{x}) \right\} d\mathbf{x}, \quad (3.1)$$

where $H_A(\mathbf{x})$ is the characteristic function of A , and we have used the standard notation $|\alpha| = \alpha_1 + \dots + \alpha_n$, $\alpha! = \alpha_1! \dots \alpha_n!$, $\mathbf{x}^\alpha = x_1^{\alpha_1} \dots x_n^{\alpha_n}$, $\mathbf{D}^\alpha = \partial^{|\alpha|} / (\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n})$.

Due to the symmetric character of the radial function, however, the regularization of a function $f(r)$ that depends only on r can be reduced to a one-dimensional problem. In fact,

$$\int_{\mathbb{R}^n} f(r) \phi(\mathbf{x}) d\mathbf{x} = \int_0^\infty f(r) \Phi(r) r^{n-1} dr, \quad (3.2)$$

where

$$\Phi(r) = r^{1-n} \int_{S_r} \phi(\mathbf{x}) d\sigma(\mathbf{x}) = \int_{S_1} \phi(r\mathbf{y}) d\sigma(\mathbf{y}), \quad (3.3)$$

S_r being the sphere of radius r and $d\sigma$ the surface measure. The function $\Phi(r)$ is defined for $r \geq 0$ only, but since all its derivatives of odd order vanish at $r = 0$, it is sometimes convenient to extend it to all $r \in \mathbb{R}$ by setting $\Phi(-r) = \Phi(r)$.

It follows that if a regularization of the function of one variable $\text{Reg}(H(r)f(r)r^{n-1})$ is given, then a regularization of $f(r)$ in $\mathcal{D}'(\mathbb{R}^n)$ can be constructed as

$$\langle \text{Reg}(f(r)), \phi(\mathbf{x}) \rangle = \langle \text{Reg}(H(r)f(r)r^{n-1}), \Phi(r) \rangle, \quad (3.4)$$

where the last operation takes place in $\mathcal{D}'(\mathbb{R}) \times \mathcal{D}(\mathbb{R})$.

Using the regularization $R_1(H(x)/x^{k-n+1})$ we obtain a regularization of $1/r^k$ that we denote as $R_n(1/r^k)$. From $Pf(H(x)/x^{k-n+1})$ we obtain the regularization $Pf(1/r^k)$, while if $\lambda + n - 1$ is not a negative integer, the canonical regularization $x_+^{\lambda+n-1}$ provides us with the canonical regularization of r^λ , which we shall denote by r_+^λ . As in the one-dimensional case, the limit of the regular part of r_+^λ when λ approaches a negative integer $-k$ with $k > n - 1$ is precisely $Pf(1/r^k)$. The regularization given by (2.25) gives rise to the regularization $\text{Reg}_A(1/r^k)$, where A is a ball of radius a and center at the origin.

When $k - n$ is odd, we have

$$\langle \delta^{(k-n)}(r), \Phi(r) \rangle = 0, \quad (3.5)$$

for any $\phi(\mathbf{x}) \in \mathcal{D}(\mathbb{R}^n)$. Therefore

$$\begin{aligned} \left\langle Pf\left(\frac{1}{r^k}\right), \phi(\mathbf{x}) \right\rangle &= \lim_{\lambda \rightarrow -k+n-1} \left\langle r_+^\lambda - \frac{(-1)^{k-n} \delta^{(k-n)}(r)}{(k-n)! (\lambda + k - n + 1)}, \Phi(r) \right\rangle \\ &= \lim_{\lambda \rightarrow -k+n-1} \langle r_+^\lambda, \Phi(r) \rangle, \end{aligned}$$

and it follows that if $n - k$ is odd the analytic function r_+^λ has a removable singularity at $\lambda = -k$, the value r_+^{-k} is thus defined and equals $Pf(r^{-k})$. Furthermore, as can be deduced from (2.15a), (2.15b), in this case the regularizations $R_n(r^{-k})$ and $Pf(r^{-k})$ coincide, too. Hence

$$r_+^{-k} = Pf(r^{-k}) = R_n(r^{-k}), \quad n - k \text{ odd}. \quad (3.6)$$

When $k - n = 2m$ is even, the analytic function r_+^λ has a simple pole at $\lambda = -k$. Since [1]

$$\Phi^{(2m)}(0) = c_{m,n} \nabla^{2m} \phi(\mathbf{0}), \quad (3.7)$$

where

$$c_{m,n} = \frac{2\Gamma(m+1/2)\pi^{(n-1)/2}}{\Gamma(m+n/2)} = \int_{S_1} y_i^{2m} d\sigma(y), \quad (3.8)$$

we find that if $k-n=2m$ is even,

$$\begin{aligned} \left\langle Pf\left(\frac{1}{r^k}\right), \phi(\mathbf{x}) \right\rangle &= \lim_{\lambda \rightarrow -k+n-1} \left\langle r_+^\lambda - \frac{(-1)^{k-n} \delta^{(k-n)}(r)}{(k-n)! (\lambda+k-n+1)}, \Phi(r) \right\rangle \\ &= \lim_{\lambda \rightarrow -k+n-1} \left[\langle r_+^\lambda, \Phi(r) \rangle - \frac{\Phi^{(2m)}(0)}{(2m)! (\lambda+k-n+1)} \right] \\ &= \lim_{\lambda \rightarrow -k+n-1} \left\langle r_+^{\lambda-n+1} - \frac{c_{m,n} \nabla^{2m} \delta(\mathbf{x})}{(2m)! (\lambda+k-n+1)}, \phi(\mathbf{x}) \right\rangle, \end{aligned}$$

or

$$Pf\left(\frac{1}{r^k}\right) = \lim_{\lambda \rightarrow -k} \left[r_+^\lambda - \frac{c_{m,n} \nabla^{2m} \delta(\mathbf{x})}{(2m)! (\lambda+k)} \right]. \quad (3.9)$$

Applying formula (2.15) it follows that if $k-n=2m$ then

$$Pf\left(\frac{1}{r^k}\right) = R_n\left(\frac{1}{r^k}\right) + \frac{(\psi(2m+1) + \gamma) c_{m,n}}{(2m)!} \nabla^{2m} \delta(\mathbf{x}). \quad (3.10)$$

Observe also that since $x^m Pf(H(x)/x^k) = Pf(H(x)/x^{k-m})$, it follows that

$$r^{2q} Pf\left(\frac{1}{r^k}\right) = Pf\left(\frac{1}{r^{k-2q}}\right). \quad (3.11)$$

When (3.10), (3.11), and the relation [1]

$$r^2 \nabla^{2m} \delta(\mathbf{x}) = (2m)(2m-2+n) \nabla^{2m-2} \delta(\mathbf{x}) \quad (3.12)$$

are used we obtain our previous result

$$\begin{aligned} r^{2q} R_n\left(\frac{1}{r^k}\right) &= R_n\left(\frac{1}{r^{k-2q}}\right) - \frac{c_{m-q,n}(\psi(2m+1) - \psi(2m-2q+1))}{(2m-2q)!} \nabla^{2m-2q} \delta(\mathbf{x}). \end{aligned} \quad (3.13)$$

The asymptotic regularization formulas can be obtained from [1] as

$$Pf\left(\frac{1}{r^k}\right) = R_n\left(\frac{1}{r^k}\right) = \lim_{\varepsilon \rightarrow 0} \left[\frac{H(r-\varepsilon)}{r^k} - \sum_{j=0}^m \frac{c_{j,n} \nabla^{2j} \delta(\mathbf{x})}{(2j)! (k-n-2j) \varepsilon^{k-n-2j}} \right], \quad (3.14)$$

if $k - n = 2m + 1$ is odd, while if $k - n = 2m$ is even we have

$$Pf\left(\frac{1}{r^k}\right) = \lim_{\varepsilon \rightarrow 0} \left[\frac{H(r - \varepsilon)}{r^k} - \sum_{k=0}^{m-1} \frac{c_{j,n} \nabla^{2j} \delta(\mathbf{x})}{(2j)! (k - n - 2j) \varepsilon^{k-n-2j}} + \frac{c_{m,n}}{(2m)!} \ln \varepsilon \nabla^{2m} f(\mathbf{x}) \right]. \quad (3.15)$$

The formulas for the derivatives of $Pf(1/r^k)$ can be derived from the corresponding formulas for $R_n(1/r^k)$ given in [1] and relation (3.10). From now on we shall assume that $k - n = 2m$ is even, since when $k - n$ is odd the derivatives do not contain extra delta function terms and thus they reduce to the ordinary derivatives.

The first derivatives of $Pf(1/r^k)$ become

$$\frac{\partial}{\partial x_i} Pf(1/r^k) = -k x_i Pf(1/r^{k+2}) - \frac{c_{m,n}}{(2m)! k} D_i \nabla^{2m} f(\mathbf{x}), \quad (3.16)$$

$$\begin{aligned} \frac{\partial^2}{\partial x_i \partial x_j} Pf(1/r^k) &= k(k+2) x_i x_j Pf\left(\frac{1}{r^{k+4}}\right) - k \delta_{ij} Pf\left(\frac{1}{r^{k+2}}\right) \\ &\quad - \frac{k c_{m+1,n}}{(2m+2)! (k+2)} \delta_{ij} \nabla^{2m+2} \delta(\mathbf{x}) \\ &\quad - \frac{c_{m,n}}{(2m)!} \left[\frac{1}{k} + \frac{1}{k+2} \right] D_{ij}^2 \nabla^{2m} \delta(\mathbf{x}). \end{aligned} \quad (3.17)$$

These results can be used even if m is negative, by setting the terms $\nabla^{2j} \delta(\mathbf{x}) = 0$ for $j < 0$. It is important to do this before any further operation is performed (for instance if $m = -1$, putting $i = j$ in (3.17) transforms the last term into $(c_{m,n}/(2m)!)(1/k + 1/(k+2)) \nabla^0 \delta(\mathbf{x})$ and a non-zero contribution would be obtained). By taking $m = -1$ in the above formulas we obtain

$$\frac{\partial}{\partial x_i} Pf\left(\frac{1}{r^{n-2}}\right) = (2-n) x_i Pf\left(\frac{1}{r^n}\right), \quad ((3.18)$$

$$\begin{aligned} \frac{\partial^2}{\partial x_i \partial x_j} Pf\left(\frac{1}{r^{n-2}}\right) &= [n(n-2) x_i x_j - (n-2) r^2 \delta_{ij}] Pf\left(\frac{1}{r^{n-2}}\right) \\ &\quad - \frac{(n-2)c_{0,n}}{n} \delta_{ij} \delta(\mathbf{x}), \end{aligned} \quad (3.19)$$

in agreement with the known formula [4].

When $m \geq 0$, by putting $i = j$ in (3.17) we obtain the formula

$$\begin{aligned}\bar{\nabla}^2 Pf(1/r^k) &= k(k+2-n) Pf(1/r^{k+2}) - \frac{c_{m,n}(k+2m+2)}{(2m)!(2m+2)k} \nabla^{2m+2} \delta(\mathbf{x}) \\ &= k(k+2-n) Pf(1/r^{k+2}) - \frac{\pi^{n/2} \nabla^{2m+2} \delta(\mathbf{x})}{2^{2m+1}(m+1)! \Gamma(m+n/2+1)},\end{aligned}$$

which agrees with the one given by Jones [3, p. 248].

In order to give the higher-order derivatives of $Pf(1/r^k)$ it is convenient to use the symmetric tensor notation. Thus, \mathbf{D}^N will denote the symmetric tensor with component $\partial^N/(\partial x_{i_1} \cdots \partial x_{i_N})$, \mathbf{x}^N the tensor with components $x_{i_1} \cdots x_{i_N}$. If S and T are symmetric tensors of order N and M then ST will denote their symmetric product, that is, the symmetrization of their tensor product $S \otimes T$; similarly, S^q will denote the symmetric product $S \cdot S \cdots S$ (q times). As usual δ will denote the Krönecker delta, a tensor of order two.

With this notation the third- and fourth-order formulas take the form

$$\begin{aligned}\bar{\mathbf{D}}^3 Pf(1/r^k) &= -k(k+2)(k+4) \mathbf{x}^3 Pf(1/r^{k+6}) + 3k(k+2) \mathbf{x} \delta Pf(1/r^{k+4}) \\ &\quad - \frac{3kc_{m+1,n}}{(2m+2)!(k+4)} \delta \mathbf{D} \Delta^{2m+2} \delta(\mathbf{x}) \\ &\quad - \frac{c_{m,n}}{(2m)!} \left(\frac{1}{k} + \frac{1}{k+2} + \frac{1}{k+4} \right) \mathbf{D}^3 \nabla^{2m} \delta(\mathbf{x}),\end{aligned}\quad (3.20)$$

$$\begin{aligned}\bar{\mathbf{D}}^4 Pf(1/r^k) &= k(k+2)(k+4)(k+6) \mathbf{x}^4 Pf(1/r^{k+8}) \\ &\quad - 6k(k+2)(k+4) \mathbf{x}^2 \delta Pf(1/r^{k+6}) \\ &\quad + 3k(k+2) \delta^2 Pf(1/r^{k+4}) \\ &\quad - \frac{3k(k+2)c_{m+2,n}}{(2m+4)!} \left(\frac{1}{k+6} - \frac{1}{k+4} \right) \delta^2 \nabla^{2m+4} \delta(\mathbf{x}) \\ &\quad - \frac{6kc_{m+1,n}}{(2m+2)!(k+6)} \delta \mathbf{D}^2 \nabla^{2m+2} \delta(\mathbf{x}) \\ &\quad - \frac{c_{m,p}}{(2m)!} \left(\frac{1}{k} + \frac{1}{k+2} + \frac{1}{k+4} + \frac{1}{k+6} \right) \mathbf{D}^4 \nabla^{2m} \delta(\mathbf{x}).\end{aligned}\quad (3.21)$$

Next let $\beta_{0,0} = 0$ and for $q \geq 1$ we set

$$\beta_{q,0} = \frac{1}{k} + \frac{1}{k+2} + \cdots + \frac{1}{k+2q-2} = \frac{1}{2} \left(\psi \left(\frac{k}{2} + q \right) - \psi(k/2) \right), \quad (3.22)$$

and define the coefficients $\beta_{q,p}$ recursively as $\beta_{0,p} = 0$ and for $q \geq 1$

$$\beta_{q,p} = \beta_{q,p-1} - \beta_{q-1,p-1}, \quad (3.23)$$

so that if $p \geq 1$

$$\begin{aligned} \beta_{q,p} &= \frac{1}{2} \sum_{j=0}^p \binom{p}{j} (-1)^j \psi\left(\frac{k}{2} + q - j\right) \\ &= \sum_{j=0}^{p-1} \binom{p-1}{j} \frac{(-1)^j}{k + 2q - 2j - 2}. \end{aligned} \quad (3.24)$$

In terms of these coefficients the formula for the N th-order derivative of $Pf(1/r^k)$ takes the form

$$\begin{aligned} \mathbf{D}^N Pf\left(\frac{1}{r^k}\right) &= \sum_{j=0}^{[N/2]} \frac{(-1)^{N-j} 2^{N-2j} \Gamma(k/2 + N - j) N!}{\Gamma(k/2) (N - 2j)! j!} \delta^j \mathbf{x}^{N-2j} Pf\left(\frac{1}{r^{k+2N-2j}}\right) \\ &\quad - \sum_{j=(|m|-m)/2}^{[N/2]} \frac{N! \Gamma(k/2 + j) c_{m+j,n} \beta_{N,j}}{(N - 2j)! \Gamma(k/2) j! (2m + 2j)!} \delta^j \mathbf{D}^{N-2j} \nabla^{2m+2} \delta(\mathbf{x}), \end{aligned} \quad (3.25)$$

where $[N/2]$ stands for the greatest integer $\leq N/2$.

Observe that formula (3.23) can be applied even if m is negative, since the lower limit in the second sum is 0 if $m \geq 0$ but becomes $|m|$ when $m \leq 0$.

In particular, the derivatives of $Pf(1/r)$ in \mathbb{R}^3 are obtained as

$$\begin{aligned} \mathbf{D}^N Pf(1/r) &= \sum_{j=0}^{[N/2]} \frac{(-1)^{N-j} 2^{N-2j} \Gamma(N - j + 1/2) N!}{\sqrt{\pi} (N - 2j)! j!} \delta^j \mathbf{x}^{N-2j} Pf\left(\frac{1}{r^{1+2N-2j}}\right) \\ &\quad - \sum_{j=1}^{[N/2]} \frac{N! \pi}{2^{2j-3} j! (j-1)! (N - 2j)!} \\ &\quad \times \sum_{q=0}^{j-1} \binom{j-1}{q} \frac{(-1)^q}{2N - 2q - 1} \delta^j \mathbf{D}^{N-2j} \nabla^{2j-2} \delta(\mathbf{x}). \end{aligned} \quad (3.26)$$

We would also like to point out that if $-\lambda - m$ is not an even integer (positive or negative), then the formulas for the derivatives of r_+^λ reduce to the ordinary ones in the sense that no extra delta terms arise. The formula then takes the form

$$\mathbf{D}^N (r_+^\lambda) = \sum_{j=0}^{[N/2]} \frac{\lambda(\lambda - 2) \cdots (\lambda - 2N + 2 + 2j) N!}{2^j j! (N - 2j)!} \mathbf{x}^{N-2j} \delta^j r_+^{\lambda - 2N + 2j}. \quad (3.27)$$

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